Chapter 6

Three-body scattering

The three-body scattering problem for short-ranged potentials below the lowest breakup threshold is logically the first challenge after the three-body bound-state problem has been solved. Thanks to the work of Faddeev, this problem poses no mysteries in either configuration space or momentum space, and it has been solved by several groups [Merkuriev *et al.*, 1976; Payne *et al.*, 1982; Chen *et al.*, 1989; Witała *et al.*, 1989]. (Many of these actually solve the breakup problem as well.) The object of this chapter is to briefly investigate the possible extension of the numerical ideas developed in the previous chapters to the three-body scattering problem.

At the time this work was done (1990), the idea of using Cartesian coordinates existed only in the back of my mind (actually, the practical problems raised by working on the three-body scattering problem helped to initiate the formation of this idea), and I therefore used polar coordinates. To avoid inessential complications, I restricted this work to the simplest possible case, that of scattering three identical particles interacting via an s-wave potential. Extensions, such as more general interactions, going above the breakup threshold, and including long-ranged potentials, should be considered in the future.

In the first section, the equations for three-body scattering below the breakup threshold are discussed. Special attention is payed to the boundary conditions. In the second section, the numerical implementation is discussed. After that, some results which I obtained using this method are shown, and compared with existing calculations. The final section contains a summary and discusses possible improvements.

6.1 Faddeev equations

As in the two-body scattering problem, the Faddeev amplitude is split into a term describing the initial state, $|\chi\rangle$, and the rest, $|\phi\rangle$, in order to be able to impose the correct boundary conditions in a convenient way:

$$|\psi_i\rangle \quad = \quad |\chi_i\rangle + |\phi_i\rangle \,. \tag{6.1}$$

Substituting this expression in the Faddeev equations and remembering that $|\chi_i\rangle$ is an eigenstate of the channel Hamiltonian H_i, we obtain

$$(E - H_i)|\phi_i\rangle \quad = \quad V_i \sum_{j \neq k} (|\phi_j\rangle + |\chi_j\rangle) \,. \tag{6.2}$$

After introducing polar coordinates and a bipolar expansion this becomes

$$\begin{aligned} & [E - H_{0i}^{\alpha} - V_i(x_i)]\phi_i^{\alpha}(\rho, \theta_i) \\ = \quad & V_i(\rho \cos\theta_i) \sum_{j \neq i} \sum_{\beta} \int_{\theta_-}^{\theta_+} \mathrm{d}\theta_j \, K_{ij}^{\alpha\beta}(\theta_i, \theta_j)[\phi_j^{\beta}(\rho, \theta_j) + \chi_j^{\beta}(\rho, \theta_j)] \,, \end{aligned} \tag{6.3}$$

where the free Hamiltonian H_{0i}^{α} is defined by Eq. (5.46), the integration limits $\theta_{\pm}$ by Eq. (5.7), and the kernel $K_{ij}^{\alpha\beta}$ by Eq. (5.9).

In the following, the discussion will be restricted to s-wave scattering for three indistinguishable particles, with precisely one two-body bound state. For that particular case, the Faddeev equations can be written as

$$\begin{aligned} & (E - H_0 - V(\rho\cos\theta))\phi(\rho, \theta) - 2V(\rho\cos\theta) \int_{\theta_-}^{\theta_+} \mathrm{d}\theta' \, \phi(\rho, \theta') \\ = \quad & 2V(\rho\cos\theta) \int_{\theta_-}^{\theta_+} \mathrm{d}\theta' \, \chi(\rho, \theta') \,, \end{aligned} \tag{6.4}$$

with

$$H_0 \quad = \quad -\frac{\partial^2}{\partial\rho^2} - \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2} \,, \tag{6.5}$$

$$\chi(\rho, \theta) \quad = \quad \psi_0(\rho\cos\theta)\hat{\jmath}_0(q\rho\sin\theta) \,, \tag{6.6}$$

where q is the momentum of the incident particle relative to the bound pair. The asymptotic boundary conditions can be derived using the asymptotic form of ϕ (cf. Eq. (4.145)):

$$\phi(\rho, \theta) \quad \underset{\rho\to\infty}{=} \quad T\psi_0(\rho\cos\theta)\hat{h}_0^{(+)}(q\rho\sin\theta) \,, \tag{6.7}$$

where T is an arbitrary constant.

6.2 Numerical solution

The three-body scattering equations differ from the bound-state equations in two ways: (*i*) there is an inhomogeneous term, and (*ii*) the boundary conditions are more complicated. We wish to apply the spline method to reduce the partial-differential equation to a matrix problem. Above all, we want to exploit as much

of the direct product structure present in the equations as possible. It is therefore necessary to investigate the effects of these differences on the matrix problem in some detail.

The inhomogeneous term changes the type of matrix problem to be solved: instead of an eigenvalue problem, it is now a set of simultaneous linear equations. Fortunately, the Lanczos method can be used successfully for such an equation as well (cf. Chapter 3). Complications due to the nontrivial boundary conditions are a little more intricate. For large ρ, the amplitude ϕ must satisfy

$$\frac{\partial}{\partial\rho}\log\phi(\rho,\theta) \approx \frac{\psi_0'(\rho\cos\theta)}{\psi_0(\rho\cos\theta)}\cos\theta + \frac{\hat{h}_0^{(+)'}(q\rho\sin\theta)}{\hat{h}_0^{(+)}(q\rho\sin\theta)}q\sin\theta\,. \tag{6.8}$$

By assuming the left-hand side to be equal to the right-hand side for ρ greater than some cutoff value $\rho_{\max}$, we obtain an approximate boundary condition. This boundary condition has an awkward form, which will cause difficulties, because it "breaks" the direct product structure: an operator working only in ρ space also has some θ dependence when discretized using the spline method. This can be seen as follows: Assuming that the ρ grid has N_ρ intervals, the last spline function in the basis for this grid, *i.e.* s_{2N_ρ}, must satisfy the boundary condition

$$s_{2N_\rho}(\rho,\theta) = \phi_{N_\rho}(\rho) + c(\theta)\xi_{N_\rho}(\rho)\,, \tag{6.9}$$

$$c(\theta) = \frac{\partial}{\partial\rho}\log\phi(\rho,\theta)\bigg|_{\rho_{\max}}\,, \tag{6.10}$$

where ξ_{N_rho} and ϕ_{N_rho} are the two spline basis functions centered around knot $k^\rho_{N_rho}$ (cf. Appendix A), which is just the end point of the interval, or, in this case, $\rho_{\max}$. The boundary condition now depends on θ, which means that the spline basis is no longer in separable form, and that the matrices representing the various operators can no longer be written as direct products.

Factorizability

The fact that the matrices representing operators cannot be written as direct products is unfortunate, since the efficiency of solving the numerical problem hinges on this structure. However, it is possible to replace the form

$$A = A_\rho \otimes A_\theta\,, \tag{6.11}$$

which can be used to represent a matrix A of a "direct-product" operator on a separable basis, by

$$A = (A_\rho \otimes \mathbb{1}_\theta + \tilde{A}_\rho \otimes \Lambda_\theta)(\mathbb{1}_\rho \otimes A_\theta)\,, \tag{6.12}$$

where $\tilde{A}$ is a rank-one correction to A_ρ, and Λ is a diagonal matrix describing the angular dependence of the boundary conditions. Such a correction can be very

easily included in most matrix operations, such as inversion (cf. Chapter 3). For example, the inverse of a matrix with a rank-m correction can be related to the inverse of the original matrix as follows:

$$(M + UV^T)^{-1} \quad = \quad \left(\mathbb{1} - M^{-1}U(\mathbb{1} + V^T M^{-1} U)^{-1} V^T\right) M^{-1}\,, \tag{6.13}$$

where M is an $n \times n$ matrix, and U and V are $n \times m$ matrices. Note that $V^T M^{-1} U$ is an $m \times m$ matrix, and can be calculated in $\mathrm{O}(nm^2)$ floating point operations. In the case of the three-body scattering problem we are dealing with rank-N corrections to $N^2 \times N^2$ matrices. These corrections basically require $\mathrm{O}(N^4)$ floating-point operations. However, if M is a sum of two direct products, this number can be reduced to $\mathrm{O}(N^3)$. Therefore, the matrix problem has essentially the same complexity as for the bound-state case, although technically it is rather more complicated.

Application of the spline method to Eq. (6.4), taking into account the changes in the basis due to the boundary conditions, leads to a matrix problem which can be written as follows (cf. Eq. (5.52)):

$$(EI - T - V - P)\boldsymbol{\phi} \quad = \quad P\boldsymbol{\chi}\,, \tag{6.14}$$

where $\boldsymbol{\phi}$ is the vector of expansion coefficients of for ϕ, and $\boldsymbol{\chi}$ is the vector of expansion coefficients for χ. The matrices I, T, V, and P are the spline matrices corresponding to the unit operator, the kinetic energy operator, the potential, and the potential multiplied with the integration operator, respectively. I will not give the matrix elements explicitly, since they are the same as for the bound-state case, with the exception that the spline basis is different, leading to numerical, not symbolic, changes. The unknown vector $\boldsymbol{\phi}$ can be calculated by inverting the matrix on the left-hand side. For reasons discussed in Chapter 5, this cannot be done directly, and therefore an iterative solution method must be applied. The Lanczos method has been shown to work very well for the two-body problem, and can be extended to the three-body problem. However, the matrix on the left-hand side does not have a small spectral radius. Guided by the experience with the bound-state problem, we rewrite the equation as follows:

$$(EI - T)^{-1}(EI - T - V - P)\boldsymbol{\phi} \quad = \quad (EI - T)^{-1} P\boldsymbol{\chi}\,. \tag{6.15}$$

The matrix on the left-hand side now has a compact spectrum, and can therefore be inverted easily using the Lanczos method. The inversion of the matrix $EI - T$ can be done using the tricks described in Chapter 5, provided the appropriate measures are taken to deal with the nonseparability, as described above. However, a reasonable rate of convergence can still be achieved by using the inverse of $E\tilde{I} - \tilde{T}$, where $\tilde{I}$ and $\tilde{T}$ are the spline representations of the unit operator and the kinetic energy operator for the bound-state problem. This leads to a significant practical simplification.

Table 6.1: Quartet scattering lengths.

	Payne	Schellingerhout
a_4 (MT-IIIa, fm)	6.442(5)	6.443(3)
a_4 (MT-Vb, fm)	14.1(5)	14.5(5)

6.3 Results

In this section, I will show some results for n–D quartet scattering, using Malfliet–Tjon model potentials (cf. Appendix B). In Table 6.1 the scattering lengths for two potentials are shown (denoted by "Schellingerhout") and compared to the values obtained by Payne *et al.* [1982] (denoted by "Payne").

My results were obtained using a 60×60 grid, which is much finer than the grid Payne used. The reason that I need a much finer grid, is that the calculations in Payne *et al.* [1982] were done by explicitly factoring out the deuteron wave function, resulting in a much smoother unknown function. However, the need for a very high number of intervals is intimately related to the use of polar coordinates, which in fact are very inefficient for the scattering problem. This can be understood as follows: Since the convergence of the Faddeev amplitude to its asymptotic form is very slow (cf. Eq. (4.145)), a very large cutoff radius (many times the range of the potential) is needed. The Faddeev amplitude has significant structure in the strip $\Omega_{\rm I} \cup \Omega_{\rm II}$ (cf. Chapter 4; the parameter R should in this case be taken to be a few times the size of the two-body bound state), but in $\Omega_{\rm II}$ it only varies rapidly with x, and is (approximately) a linear function of y. When Cartesian coordinates are used, this can be exploited, by subdividing the y grid into an inner part having small intervals, and an outer part having much larger intervals. Consequently, the number of intervals is virtually independent of the value of $\rho_{\rm max}$. When, on the other hand, polar coordinates are used, the situation changes drastically. For large values of ρ and small values of x, we have approximately

$$\theta \quad = \quad \frac{\pi}{2} - \frac{x}{\rho}\,, \tag{6.16}$$

which means that the size of the intervals in the θ grid near $\frac{\pi}{2}$ must be of the order $h/\rho_{\rm max}$, where h is grid size in the x direction needed to describe the x dependence accurately. This means that the number of intervals in the θ grid must be of the order of $\rho_{\rm max}/h$, so that the number of intervals increases rapidly with $\rho_{\rm max}$. (Note that for the bound-state case this is not a real problem, since for that case the Faddeev amplitude decreases exponentially, and $\rho_{\rm max}$ can be taken rather small.)

Note that the MT-Vb result is rather uncertain, since the required cutoff radius

Table 6.2: Quartet phase shifts for the MT-IIIa potential.

E_{cm} (MeV)	Chen	Schellingerhout
0.001	−2.09	−2.09(1)
0.050	−14.6	−14.6(1)
1.000	−55.8	−55.9(1)
1.633	−66.7	−66.7(1)
2.180	−73.6	−73.5(1)

is very large. My result is based on a cutoff radius of 100 fm instead of the 60 fm used for the MT-IIIa result.

In Table 6.2 some quartet phase shifts (in degrees) for the MT-IIIa potential are given (denoted by "Schellingerhout"), and compared to the results of Chen *et al.* [1989] (denoted by "Chen"). My results were obtained using a 40×40 grid.

6.4 Conclusion

I have shown that the ideas developed in the previous chapters can be extended to the three-body scattering problem below the breakup threshold. The additional problems are of a technical nature and can be solved without loss of numerical efficiency. I have compared my results with other calculations using a different method, and found near perfect agreement.

The method described here can be extended easily to involve more channels. Below the breakup threshold, the extension to long-ranged forces is not very difficult. More general interactions can also be included with relative ease. Difficulties can be expected above the breakup threshold, because of two reasons. The first reason is that the boundary conditions become more difficult to implement, and the second is that the Faddeev amplitude no longer decreases exponentially in any direction. This implies that an even larger cutoff radius might be necessary.

Improvements can be made, such as introducing Cartesian coordinates. This will lead to a better capacity for coping with the nonvanishing structure for small values of x when y goes to infinity. Also, it is of interest to see if the method described in Chapter 4 — implementing the boundary conditions in an exact manner at very small radius using a one-dimensional integral equation — can be applied in practice, in an efficient manner.